Spectral Portait Computation by a Lanczos Method

(Normal Equation version)

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Abstract

This work describes a software tool intended for the evaluation of spectral portraits of nonsymmetric matrices. This requires to compute the 2-norm of the matrix $(A - zI)^{-1}$, for points z in a discretized region of the complex plane. In order to estimate this 2-norm, i.e, the smallest singular value of $(A - zI)$, a Lanczos procedure is applied to the operator $(A - zI)^*(A - zI)$, which corresponds to a normal equation formulation. The importance and fundamentals of spectral portraits are first reviewed. Then, we describe the sequence of operations required for their evaluation, including the estimation of the smallest singular value by means of an eigenproblem approach, possible strategies to speed up the computation and implementation details. Next, we give a wide range of study cases as a way to result a critical analysis of the methodology employed and to define guide-lines for future activities. Finally, a user's guide is given, with a description of the required input and output files.

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Contents

1 Introduction

Eigenvalue computations are very important for the study of the stability of physical problems. However, in finite precision arithmetic, some problems may occur in the computation of eigenvalues related with highly nonnormal operators.
Tests performed with matrices for which the departure from normality is parametrized, show that the QR method converges to eigenvalues far away from the exact solutions. For some problems in physics, for instance, one must be sure that all the eigenvalues have a negative real part. If the associated operator is nonnormal, the real part of some computed eigenvalues may become positive. How can one interpret such behaviour? On the other hand, Trefethen has shown that in hydrodynamics, the utilisation of perturbed operators may lead, in several cases, to results matching those of physical experiments.
Therefore, the question is : How does a perturbation affect an eigenvalue?
A possible answer is given by the condition number, which can be computed for simple eigenvalues, but in the case of defective multiple eigenvalues only an upper bound exists. Therefore, the classical tools turn out to be inefficient.
In order to overcome this inefficiency, one should examine the eigenvalues of $A + \Delta A$ and not only those of A. Thus, let us define an ε-pseudoeigenvalue and an ε-pseudospectrum of A :

- λ is an ε-pseudoeigenvalue of A if

$$\lambda \text{ is an eigenvalue of } A + E \text{ with } \|E\|_2 \leq \varepsilon \|A\|_2$$

- The ε-pseudospectrum of A is defined by

$$\Lambda_\varepsilon(A) = \{z \in \mathbb{C}; z \text{ is an } \varepsilon\text{−pseudoeigenvalue of } A\}$$

We will see in the next section that, for a fixed ε, the border of $\Lambda_\varepsilon(A)$ can be defined as $\{z \in \mathbb{C}; \|A\|_2 \|(A - zI)^{-1}\|_2 = \frac{1}{\varepsilon}\}$.

Godunov (Godunov (1991)) calls the graphical representation of

$$z \longrightarrow log_{10}(\|A\|_2 \|(A - zI)^{-1}\|_2)$$

the **spectral portrait** of A.
Unlike the condition number, which is a first order estimation and allows the study of the singularity only in a circle with radius tending to 0 (asymptotic behaviour), the spectral portrait allows the study of the influence of the singularity in a larger topological neighbourhood.

2 Notations

x^* is the conjugate transpose vector of x. A^* is the conjugate transpose matrix of A. Throughout this document, we use the following notations :

A	real nonsymmetric matrix
$sp(A)$	spectrum of A
n	dimension of A
z_1	lower left point of the discretized space
z_2	higher right point of the discretized space
$xmesh$	number of discretization points on the real axis
$ymesh$	number of discretization points on the complex axis
tol	threshold for convergence (backward error)
p	number of required eigenpairs
m	maximal number of steps
z	point in the discretized complex plane
$\mathcal{H}_n(z)$	hermitian matrix defined as $(A - zI)^*(A - zI)$
$\{\sigma(z)_i\}_{i=1}^n$	singular values of $(A - zI)$
$\{\lambda(z)_i\}_{i=1}^n$	eigenvalues of $\mathcal{H}_n(z)$
$\{x(z)_i\}_{i=1}^n$	eigenvectors of $\mathcal{H}_n(z)$
$Q(z)_j$	Lanczos basis at j^{th} step
$\{q(z)_i\}_{i=1}^j$	vectors of the Lanczos basis at j^{th} step
$T(z)_j$	tridiagonal matrix defined as $T(z)_j = Q(z)_j^* \mathcal{H}_n(z) Q(z)_j$
$\{y(z)_i\}_{i=1}^j$	eigenvectors of $T(z)_j$
$\{\theta(z)_i\}_{i=1}^j$	eigenvalues of $T(z)_j$

For the sake of simplicity, we shall write Q_j, T_j, ... instead of $Q(z)_j$, $T(z)_j$, ... when no confusion is possible.

3 Spectral portrait description

By means of Turing's theorem, one can show that $\{z \in \mathbb{C}; z$ is an eigenvalue of $A + \Delta A;\ \|\Delta A\|_2 \leq \varepsilon \|A\|_2\}$ is equivalent to $\{z \in \mathbb{C};\ \|(A - zI)^{-1}\|_2 \|A\|_2 \geq \frac{1}{\varepsilon}\}$. The proof can be found in Trefethen.

Therefore, to compute a spectral portrait, the main problem consists in the evaluation of

$$z \longrightarrow \|(A - zI)^{-1}\|_2 \text{ for } z \in \mathbb{C} \ . \qquad (1)$$

We recall that $\|B\|_2 = \sigma_{max}(B)$ and $\|B^{-1}\|_2 = \dfrac{1}{\sigma_{min}(B)}$ where B is an $n \times n$ matrix and $\{\sigma_i(B)\}_{i=1}^n$ its singular values. We denote $\sigma_{min}(B)$ (resp. $\sigma_{max}(B)$) the smallest (resp. the largest) singular value of B.

Therefore, the equation (1) can be rewritten as :

$$z \longrightarrow \frac{1}{\sigma_{min}(A - zI)} = \|(A - zI)^{-1}\|_2 \tag{2}$$

which requires the determination of the smallest singular value of a matrix.

The evaluation of (2) can be performed in different ways. We present three of them, namely singular value decomposition (SVD), Normal Equation method and Augmented Matrix method, and give their respective condition numbers $CN(svd)$, $CN(ne)$ and $CN(am)$. Since the SVD method will be used as a reference technique, we compare its conditioning with the other two.

a) Singular Value Decomposition :

This method (see Golub and Van Loan (1989)) is very reliable but computationally expensive. The condition number of this method is denoted by $CN(svd)$ and is

$$CN(svd) = \frac{\|B\|_2}{\sigma_{min}(B)}.$$

Proof :

$$CN(svd) = \lim_{\varepsilon \longrightarrow 0} \left[\frac{|\sigma_{min}(B + \Delta B) - \sigma_{min}(B)|}{\sigma_{min}(B)} \times \frac{\|B\|_2}{\|\Delta B\|_2} \right]$$

but (see Golub and Van Loan (1989, page 428))

$$|\sigma_{min}(B + \Delta B) - \sigma_{min}(B)| \;\leq\; \sigma_{max}(\Delta B) \;=\; \|\Delta B\|_2$$

and

$$\frac{1}{\sigma_{min}(B)} \;=\; \|B^{-1}\|_2$$

thus

$$CN(svd) = \|B^{-1}\|_2 \|B\|_2 = \frac{\|B\|_2}{\sigma_{min}(B)}$$

□

b) Normal Equation method :

We compute $\sigma_{min}(B)$ in the following way :

$$\sigma_{min}(B) = \sqrt{\lambda_{min}(B^* B)}\ .$$

We call this method, the "Normal Equation method", in analogy with the least squares problem $min\|Ax-b\|$ which can be reformulated as a linear system $A^*Ax = A^*b$.
The computation of a singular value is replaced by the computation of an eigenvalue of B^*B. Using a projection method allows us to work with larger matrices. The drawback is that the condition number, denoted now $CN(ne)$, is such that

$$CN(ne) \sim (CN(svd))^2 \; .$$

Proof :

We can find in Chatelin (1988) that

$$CN(ne) = \frac{\|B^*B\|_2\|x_*\|_2\|x\|_2}{|x_*x||\lambda_{min}(B^*B)|} \; ,$$

where x (resp. x_*) is the right (resp. left) eigenvector of B^*B corresponding to $\lambda_{min}(B^*B)$. Since B^*B is hermitian, we have $x_* = x$ and $\|x\|_2 = 1$.

Thus, we can write :

$$CN(ne) = \frac{\|B^*B\|_2}{|\lambda_{min}(B^*B)|} \leq \frac{\|B\|_2^2}{(\sigma_{min}(B))^2} = (CN(svd))^2 \; .$$

□

c) Augmented Matrix method :

This method is based on the use of $\begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix}$ denoted by $\mathcal{B}_a$, to compute the singular values of B.
Indeed, recalling that $sp(B^*B) = \{(\sigma_1(B))^2, (\sigma_2(B))^2, ..., (\sigma_n(B))^2\}$, one can write

$$sp(\mathcal{B}_a) = \{-\sigma_n(B), ..., -\sigma_1(B), +\sigma_1(B), ..., +\sigma_n(B)\}$$

Thus, to determine $\|B^{-1}\|_2$, we have to compute $|\sigma_1(B)|$ which is an eigenvalue of the matrix $\mathcal{B}_a$.

This method works with a matrix whose size is twice as large as the corresponding matrices of the other two methods. However, we can benefit from the block strucure of $\mathcal{B}_a$ and its hermitian property.
Furthermore, it can be checked that for the third condition number denoted $CN(am)$,

$$CN(am) \leq \sqrt{2}\sqrt{n}\; CN(svd) \; .$$

Proof :

The condition number of the eigenvalue $\lambda_{min}(\mathcal{B}_a) = |\sigma_1(B)|$ is

$$CN(am) = \frac{\|\mathcal{B}_a\|_2 \ \|x_*\| \|x\|}{|\lambda_1(\mathcal{B}_a)| \ |x_* x|} ,$$

where x (resp. x_*) is the right (resp. left) eigenvector of $\mathcal{B}_a$ corresponding to $\lambda_1(\mathcal{B}_a)$ Since $\mathcal{B}_a$ is hermitian, we have $x_* = x$ and $\|x\|_2 = 1$.

Thus, we can write

$$CN(am) = \frac{\|\mathcal{B}_a\|_2}{|\sigma_1(\mathcal{B}_a)|}$$

but

$$\|\mathcal{B}_a\|_F^2 = \sum_{i,j} b_{ij}^2 + \sum_{i,j} b_{ij}^{*2} = \|B\|_F^2 + \|B^*\|_F^2 = 2\|B\|_F^2 \ .$$

Because $\|B\|_F \leq \sqrt{n}\|B\|_2$, one can write $\|\mathcal{B}_a\|_2 \leq \sqrt{2}\sqrt{n}\|B\|_2$ and

$$CN(am) \leq \frac{\sqrt{2}\sqrt{n}\|B\|_2}{|\lambda_1(\mathcal{B}_a)|} \leq \frac{\sqrt{2}\sqrt{n}\|B\|_2}{\sigma_{min}(B)} \leq \sqrt{2}\sqrt{n} \ CN(svd) \ .$$

□

Therefore, we have shown that the Normal Equation method may have a strong ill conditioning. However, in this report, we develop this method as a first approach for spectral portrait evaluations in order to enlight its numerical difficulties. This will justify the examination of the Augmented Matrix method, which will be fully described in a forthcoming report.

The method chosen to compute $\lambda_{min}[(A - zI)^*(A - zI)]$ is based on the Lanczos method, which is very appropriate for computing the extreme eigenvalues of hermitian matrices.
Common implementations of the Lanczos algorithm require the user to provide the matrix-vector product. Here this product is $(A - zI)^*(A - zI)x$.

Thus, our work consists in :

- discretizing the complex plane

- computing, for each point z

$$\begin{aligned} z \longrightarrow \phi(z) &= log_{10}(\|A\|_2\|(A-zI)^{-1}\|_2) \\ &= log_{10}[\lambda_{max}(A^*A)\lambda_{min}((A-zI)^*(A-zI))]^{-\frac{1}{2}} \ . \end{aligned}$$

Because the variations of $\|(A-zI)^{-1}\|_2$ in the neighbourhood of an eigenvalue are extremely stiff, the level curves of $z \longrightarrow \|A\|_2\|(A-zI)^{-1}\|_2$ corresponding to a uniform scale are not very informative. To circumvent this difficulty, we can use rather an **exponential** scale, which amounts to a uniform scale for $z \longrightarrow \phi(z)$.

4 Spectral portrait computation

In this section we examine the sequence of operations required for the evaluation of a spectral portrait. First we define the variables that we use in our computation. Then we list the steps to determine the spectral portrait, as well as the algorithm used to estimate the required eigenvalues. Finally, we present the strategies and versions implemented to improve the computational performance.

4.1 Spectral portrait determination

The basic steps required for the determination of the spectral portrait are described below

- Step 1. Define a region of the complex plane by z_1 and z_2.
- Step 2. Discretize the region by *xmesh* and *ymesh*.
- Step 3. For each point z of the discretized region, compute $\|(A-zI)^{-1}\|_2$.
- Step 4. Graphical processing using *Matlab*.

In order to define the region to be studied, we recall that each eigenvalue λ of A satisfies $|\lambda| \leq \|A\|_2$. Thus, for a global analysis of the spectrum, the region under study must contain more than the disk $(0, \|A\|_2)$ because of the possible diffusion of some eigenvalues outside the spectrum (see Figure 6).

The discretized region is used as shown in Figure 1. The motivation of this choice will become clear in section 3.3.4 .
The computation of $\phi(z)$ requires the determination of $\lambda_{max}(A^*A)$ and
$\lambda_{min}((A-zI)^*(A-zI))$, which will be examined in the next section.

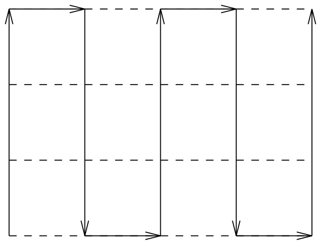

Figure 1: The spectral portrait computational path.

4.2 Eigenvalue computation

The technique used for the computation of the eigenvalues (i.e. λ_{min} and λ_{max}) is based on a Lanczos method applied to $\mathcal{H}_n(z) = (A - zI)^*(A - zI)$. We use the subroutine HLDRVS, which is described in Marques (1994). Some important characteristics of this code are given below.

4.2.1 Generalities

The unique routine, HLDRVS sets values for control parameters, computes some eigenvalues of $\mathcal{H}_n(z)$ (usually the extreme ones) and, if required, the associated eigenvectors. The algorithm used by HLDRVS requires the multiplication of a vector by the matrix $\mathcal{H}_n(z)$, until the convergence for the prescribed number of solutions is reached. However, every time a matrix-vector multiplication has to be performed, the control is returned to the user (reverse communication strategy). Thus, the matrix $\mathcal{H}_n(z)$ does not have to be passed as an argument.

4.2.2 Method

The algorithm used by HLDRVS is based on the Lanczos method, in combination with a modified partial reorthogonalization strategy.

The basic idea consists in the generation of a Krylov basis of vectors $Q_j = [q_1, ..., q_j]$, with $j < n$, such that the projection of $\mathcal{H}_n(z)$ into Q_j leads to a reduced problem, i.e,

$$Q_j^* \mathcal{H}_n(z) Q_j = T_j$$

where T_j is a symmetric tridiagonal matrix.

Assuming that (θ, y) is an exact eigensolution of the reduced problem, $(\theta, Q_j y)$ is an approximate solution of the original one. We define as $(\tilde{\lambda}, \tilde{x})$ the pair $(\theta, Q_j y)$ computed *in finite arithmetic precision.*

The algorithm is summarized below

```
1. Initialization:

   set $q_0 = 0$ and $\beta_1 = 0$
   set $q_1 \neq 0$ so that $q_1^* q_1 = 1$

2. Lanczos steps:

   for j=1,2,... m

      a) $r_j \leftarrow \mathcal{H}_n(z) q_j$
      b) $r_j \leftarrow r_j - q_{j-1}\beta_j$
      c) $\alpha_j \leftarrow q_j^* r_j$
      d) $r_j \leftarrow r_j - q_j \alpha_j$
      e) $\beta_{j+1} \leftarrow \sqrt{r_j^* r_j}$
      f) $q_{j+1} \leftarrow \frac{1}{\beta_{j+1}} r_j$
      g) if required orthogonalize $q_j$ and $q_{j+1}$ against the vectors of $Q_{j-1}$
      h) insert $q_j$ into $Q_j$, $t_{j,j-1} \leftarrow \beta_j$, $t_{j-1,j} \leftarrow \beta_j$, $t_{j,j} \leftarrow \alpha_j$
      i ) solve the reduced problem $T_j y_k = y_k \theta_k$
      j ) check $nc$, the number of eigenpairs for which
         $\|\mathcal{H}_n(z)\tilde{x} - \tilde{\lambda}\tilde{x}\|_2 = \|\beta_{j+1} y_j^{(k)}\|_2 \leq tol \; \|\mathcal{H}_n(z)\|_2$

      If $nc \geq p$, exit.

3. Compute the eigenvector approximations (related with $nc$):

      $\tilde{x}_k = Q_j y_k$
```

4.2.3 Stopping criterion

The stopping criterion is based on the backward error analysis. The backward error related to the i^{th} computed eigenpair $(\tilde{\lambda}_i, \tilde{x}_i)$ is given by

$$\eta(z)_i = \frac{\|\mathcal{H}_n(z)\tilde{x}_i - \tilde{\lambda}_i \tilde{x}_i\|_2}{\|\mathcal{H}_n(z)\|_2} \; .$$

The numerator can be computed using information provided by the Lanczos code[1]. Indeed, at the j^{th} step of the algorithm, we have :

$$\|\mathcal{H}_n(z)\tilde{x}_i - \tilde{\lambda}_i \tilde{x}_i\|_2 = \beta_{j+1}|y_i^{(j)}| \; ,$$

[1] provided that $\frac{\beta_{j+1}|y_i^{(j)}|}{\|\mathcal{H}_n(z)\|_2} \geq$ *machine precision* . See Bennani and Braconnier (1993b).

where β_{j+1} is the normalizing factor associated with the $(j+1)^{th}$ Lanczos vector and $y_i^{(j)}$ is the last component of the eigenvector related to the i^{th} eigenvalue of the reduced problem.
Since $\mathcal{H}_n(z)$ is hermitian, $\|\mathcal{H}_n(z)\|_2 = \lambda_{max}(\mathcal{H}_n(z))$, which is also obtained during the computation because Lanczos usually approaches both minimal and maximal eigenvalues.

4.2.4 Versions and strategies

We have implemented two versions, which differ in the choice of q_1, the first eigenvector of the Lanczos basis.

- For the *general version*, at each point we use as starting vector
$$q_1 = \frac{1}{\sqrt{n}}(1,\ 1,\ \ldots 1)^*\ .$$
- For the *previous point version*, if we define z_{l+1} as the point after z_l in the discretization, we use as starting vector
$$q_1 = \tilde{x}_1(z_l)/\|\tilde{x}_1(z_l)\|_2\ ,$$
where $\tilde{x}_1(z_l)$ is the eigenvector associated with the smallest eigenvalue of $\mathcal{H}_n(z_l)$.

The previous point version was implemented in order to reduce the basis size, required for the convergence to λ_{min}.
Although it seems very attractive, this approach is not always reliable, as we will see in the examples. In addition, both versions use a restarting strategy : when the basis size reaches the maximal number of steps allowed, m, and the convergence of λ_{min} was not reached, the Lanczos code is restarted taking
$$q_1 = \frac{\tilde{x}_1(z)}{\|\tilde{x}_1(z)\|_2}$$
as starting vector.

4.2.5 Implementation details

It should be noted that the sparsity of the matrix is not taken into account. As it can be seen in the *User's Guide* section, `portrait` can deal with matrices from the Harwell-Boeing collection(Duff, Grimes, and Lewis (1992)). For the input of the matrices, we use the subroutine `readmt` from the *SPARSKIT* library (Saad (1993)) but, as mentioned before, such matrices are stored as dense.
On the other hand, the spectral portraits for the Harwell-Boeing matrices are computed using only the *previous point version.*

5 Numerical results

In this section, we will first validate the proposed techniques on matrices already treated in Carpraux, Erhel, and Sadkane (1993), namely Godunov and HOR131 from the Harwell-Boeing collection. Then, we will use two other matrices to show the different problems that one can meet using the code. Finally, we give a comparison in terms of the CPU time required by our techniques and the SVD .

5.1 Description of the Figures

Before presenting the numerical results, in Table 1 we list the characteristics of the problems examined and the corresponding figures.

Figure	Matrix	Size	Method	Parameters			
				All methods	Normal Equation method		
				Mesh	m	p	tol
2	Godunov	7	SVD	256×256			
3	Godunov	7	General	256×256	5	3	10^{-12}
4	Godunov	7	Previous Point	256×256	4	2	10^{-12}
5	HOR131	434	Harwell-Boeing	200×50	100	45	10^{-08}
6	La Rose	10	SVD	256×256			
7	La Rose	10	General	256×256	7	5	10^{-15}
8	La Rose	10	Previous Point	256×256	6	4	10^{-15}
9	Tolosa	135	SVD	256×256			
10	Tolosa	135	General	128×128	80	55	10^{-12}
11	Tolosa	135	Previous Point	256×256	50	25	10^{-15}
12	Tolosa	135	Previous Point	100×100	80	60	10^{-15}
13	Tolosa	135	General	10×10	70	50	10^{-15}
14	Tolosa	135	Previous Point	10×10	70	50	10^{-15}

Table 1: Description of the Figures.

5.2 Matrices studied

5.2.1 Godunov matrix

This matrix was introduced by Godunov and its spectral portrait was previously studied in Carpraux, Erhel, and Sadkane (1993). The matrix is defined by

$$A = \begin{pmatrix} -2 & 25 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3 & 10 & 3 & 3 & 3 & 0 \\ 0 & 0 & 2 & 15 & 3 & 3 & 0 \\ 0 & 0 & 0 & 0 & 15 & 3 & 0 \\ 0 & 0 & 0 & 0 & 3 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 25 \\ 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}$$

so that, the eigenvalues correspond to $\{-3, -2, 0, 2, 3\}$ with -3 and -2 of multiplicity 2.
An analysis of the Figures 2, 3 and 4 shows a good behaviour of both previous point and general versions in comparison with the SVD method.
The neighbourhood of the eigenvalues -3 and -2 can be considered as ill conditionned because of the collective behaviour observed in this region.

5.2.2 Harwell-Boeing matrix

The matrix HOR131, of dimension 434, has 4710 entries and is related with a flow network problem. Its spectral portrait was studied in Carpraux, Erhel, and Sadkane (1993).
As we can see in Figure 5, the spectrum of HOR131 can be as stable because the largest value on the scale of the spectral portrait is moderate. Therefore, perturbations less than or equal to 10^{-6} do not lead to significant changes in its eigenvalues.

5.2.3 La Rose matrix

The matrix called La Rose is the companion matrix associated with the polynomial $P(x) = (x-1)^3(x-2)^3(x-3)^3(x-4)$.

It is defined by

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -864 & 4968 & -12492 & 18086 & -16703 & 10290 & -4287 & 1194 & -213 & 22 \end{pmatrix}$$

so that its spectrum has one simple eigenvalue, equal to 4, and three defective eigenvalues of multiplicity 3 : $1, 2$ and 3 respectively. Considering these multiplicities, the spectrum is difficult to compute.

The analysis of the figures 6, 7 and 8 shows a good general evaluation of the spectral portrait obtained with both general and previous point versions in comparison with the SVD method.
We can observe a collective behaviour mainly in the neighbourhood of the eigenvalues 2 and 3.
However, the general and previous point versions present a pigmentation around those eigenvalues that does not appear with the SVD method. Some preliminary tests with the Augmented Matrix strategy have not shown this phenomenon, which seems to be related with the condition number of the Normal Equation approach. For example, when using the expression for $CN(c)$ introduced in section 3 for the point $(2.01, 0)$ and $(2.0001, 0)$, we get condition numbers of order 10^{38} and 10^{42}, respectively.

The next application will illustrate the problems we can meet with the previous point version.

5.2.4 Tolosa135 matrix

This matrix has dimension 135 and was provided by engineers from *Aerospatiale*, who wanted to compute the eigenvalues with largest imaginary part. The matrix is associated with a flutter analysis problem (Braconnier, Chatelin, and Dunyach (1995)).

An examination of the results shows an agreement between the general version, Figure 10 and the SVD method, Figure 9. However, the previous point version does not show a large part of the spectrum, as can be seen in Figure 11.
This problem might be related to : a) the size of the basis generated by the Lanczos algorithm, b) a starting vector orthogonal to the eigenvector associated with the smallest eigenvalue.

The spectral portrait shown in Figure 12 was also computed using the previous point version, but with a basis size larger than the one for Figure 11. We obtain a better representation of the spectrum, although we can observe vertical perturbations. These perturbations can be explained by focussing on a small region of the plane, as shown in Figures 13 and 14 obtained by computed the spectral portrait with a 10×10 mesh. Considering the spectral portrait computational path (see Figure 1), the first five points are correct with the previous point version. For the subsequent points, the computation is not accurate.

This problem is related with the starting vector supplied to the Lanczos algorithm. Actually, for the point $z_1 = (-50, 170)$, we find with both general and previous point versions $\lambda_{min}(\mathcal{H}_n(z_1)) = 4.3539 \times 10^{-2}$. Taking as starting vector for the next point $z_2 = (-50, 174)$ the eigenvector associated with 4.3539×10^{-2}, the previous point version obtains $\lambda_{min}(\mathcal{H}_n(z_2)) = 3.2072 \times 10^{-2}$, which is in fact the second eigenvalue of $\mathcal{H}_n(z_2)$, the smallest being 3.1225×10^{-2}. The convergence could not be reached with the basis size we used, because the starting vector is orthogonal to the eigenvector associated with the eigenvalue 3.1225×10^{-2}. This phenomenon may continue for consecutive points and independently of the characteristics of the matrix (nonnormality, norm ...). Therefore, the previous point version is not a reliable strategy for the spectral portrait evaluation. On the other hand, the general version uses always the starting vector $u/\|u\|_2$, where $u = ((1,0), (1,0), ..., (1,0))^T$, and does not suffer from the aforementioned problem.

5.3 Figures

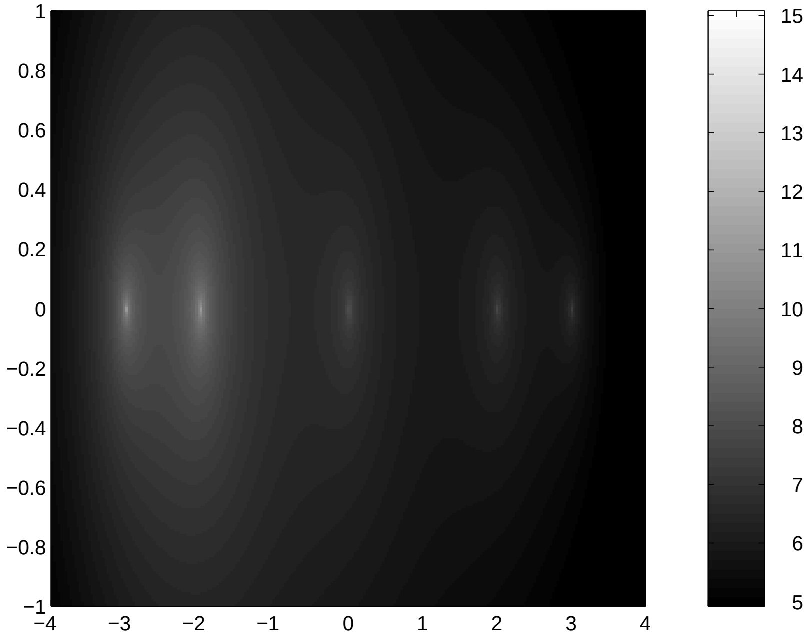

Figure 2: Godunov matrix. SVD method.

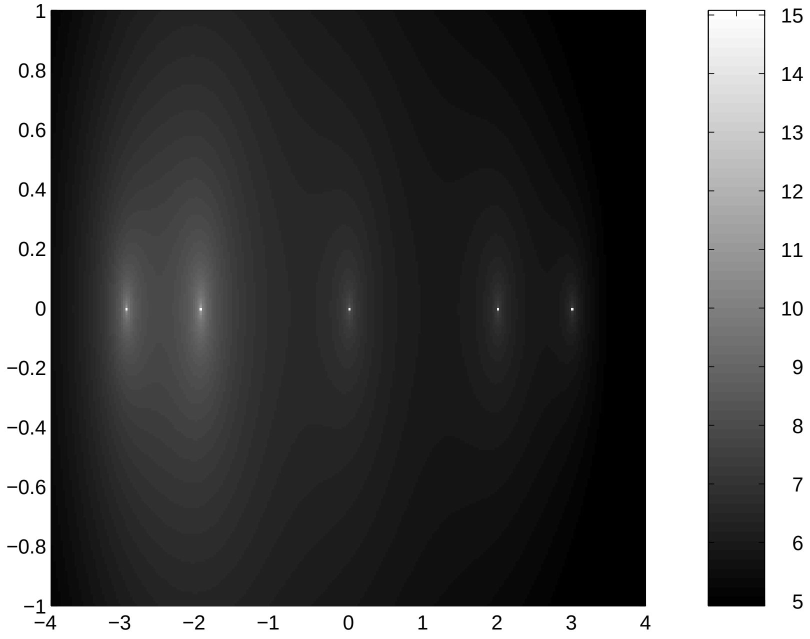

Figure 3: Godunov matrix. General version.

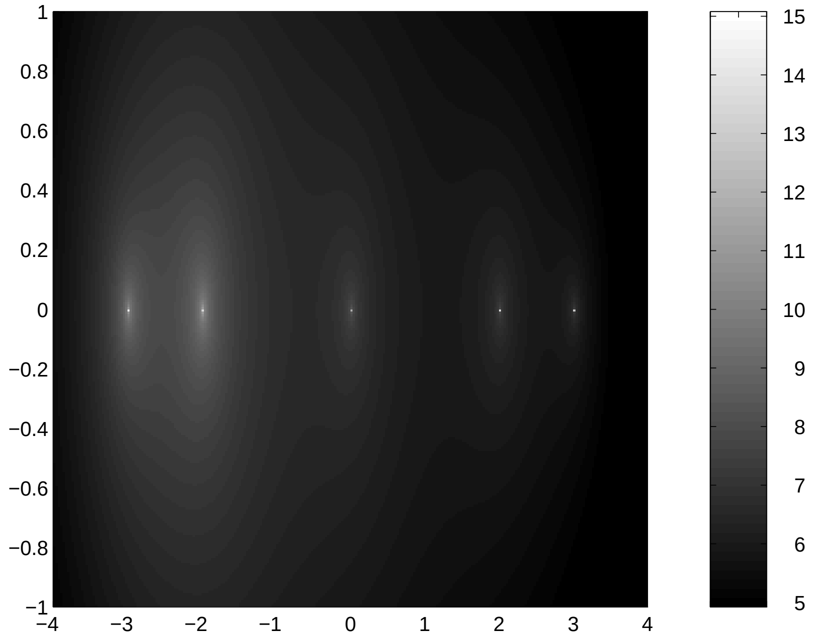

Figure 4: Godunov matrix. Previous Point version.

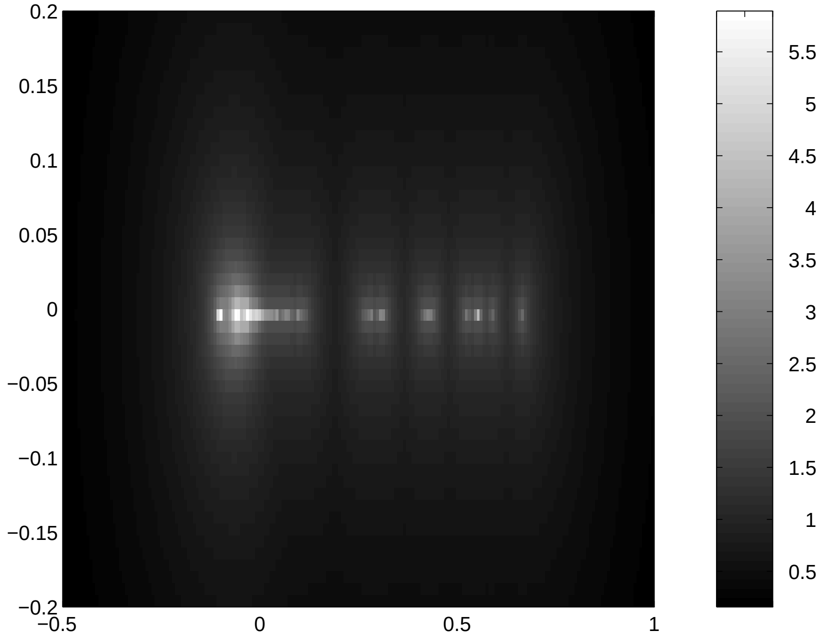

Figure 5: HOR131 matrix. Previous Point version.

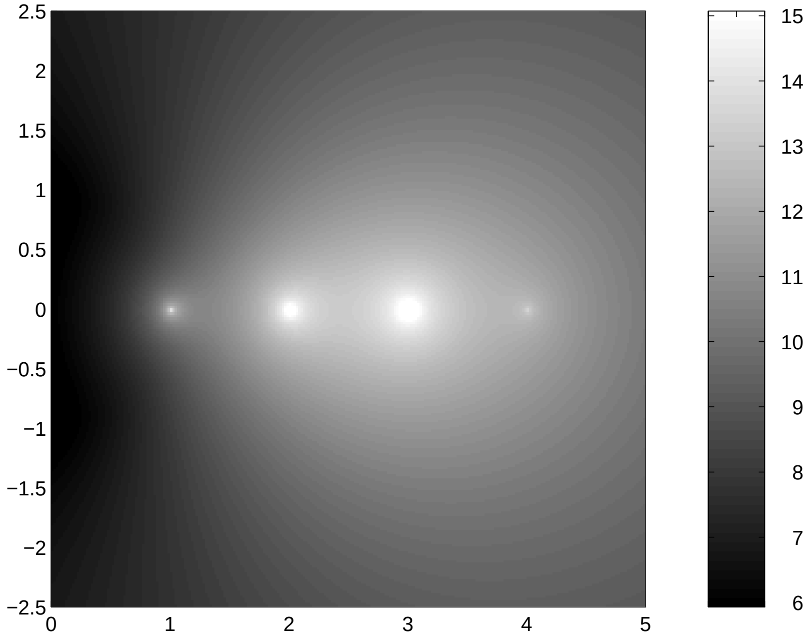

Figure 6: La Rose matrix. SVD method.

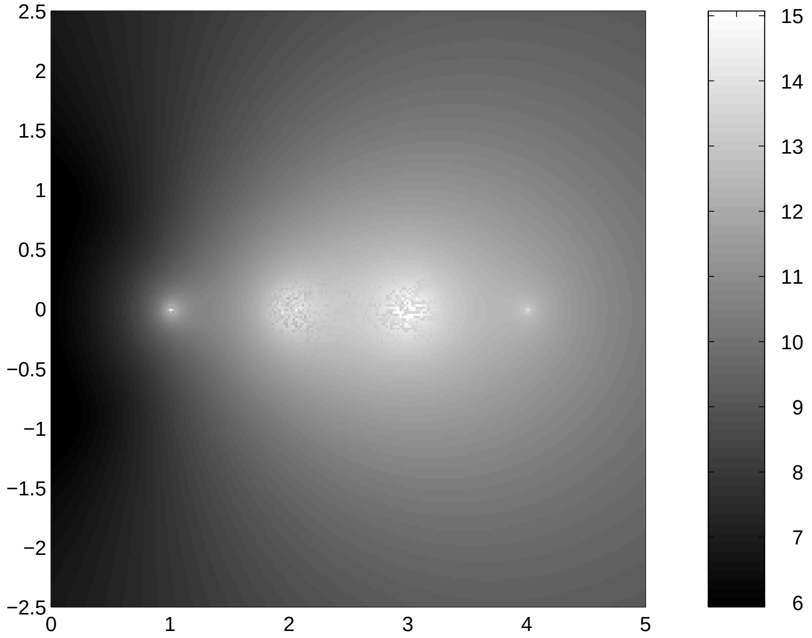

Figure 7: La Rose matrix. General version.

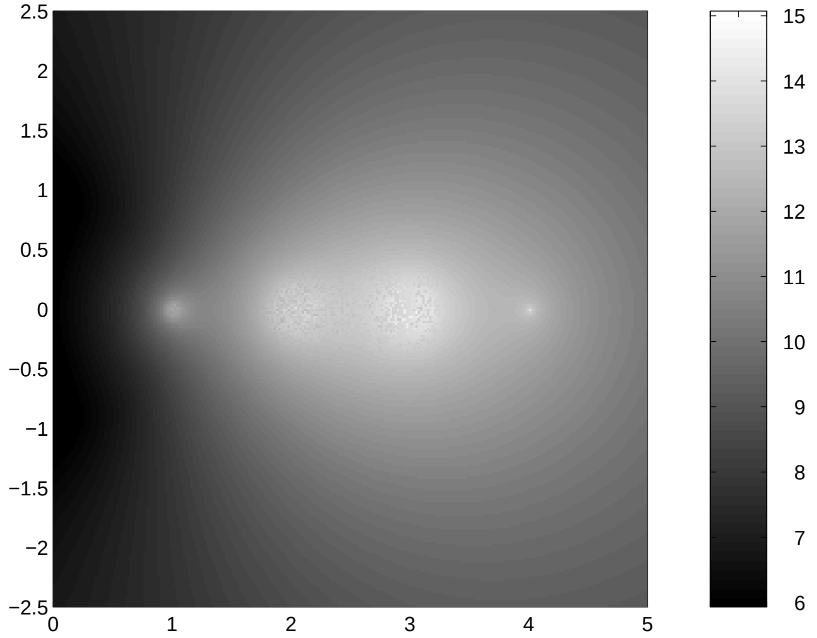

Figure 8: La Rose matrix. Previous Point version.

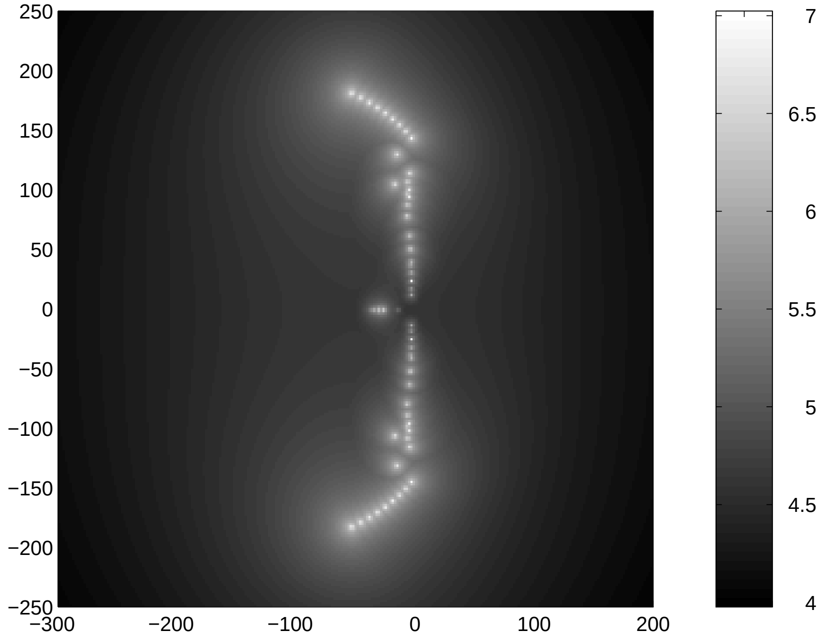

Figure 9: Tolosa matrix. SVD method.

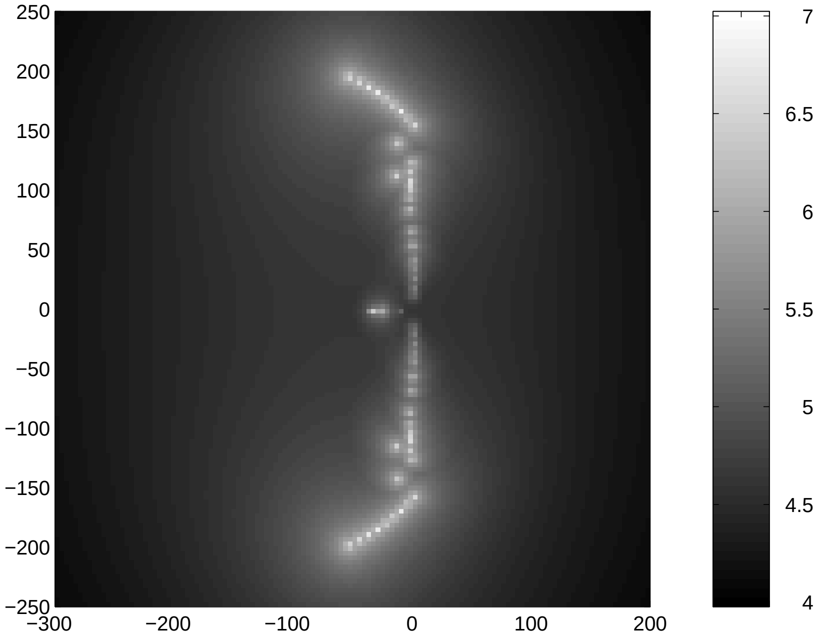

Figure 10: Tolosa matrix. General version.

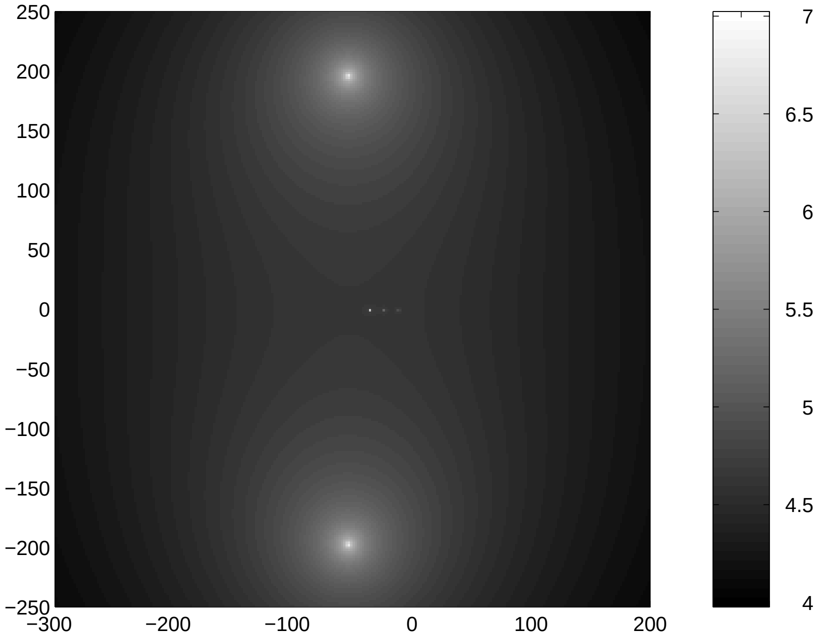

Figure 11: Tolosa matrix. Previous Point version. Orthogonality problem. $m = 50,\ p = 25$

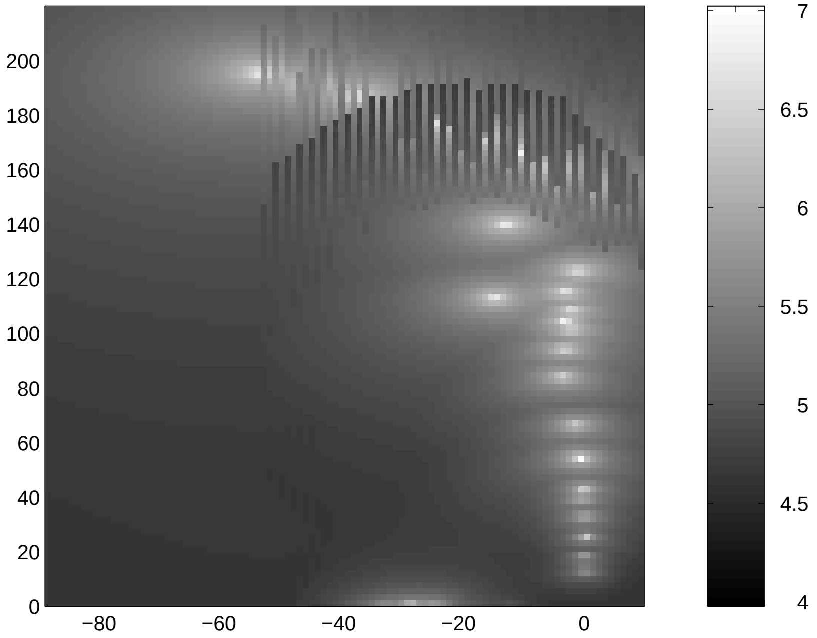

Figure 12: Tolosa matrix. Previous Point version. Orthogonality problem. $m = 80,\ p = 60$

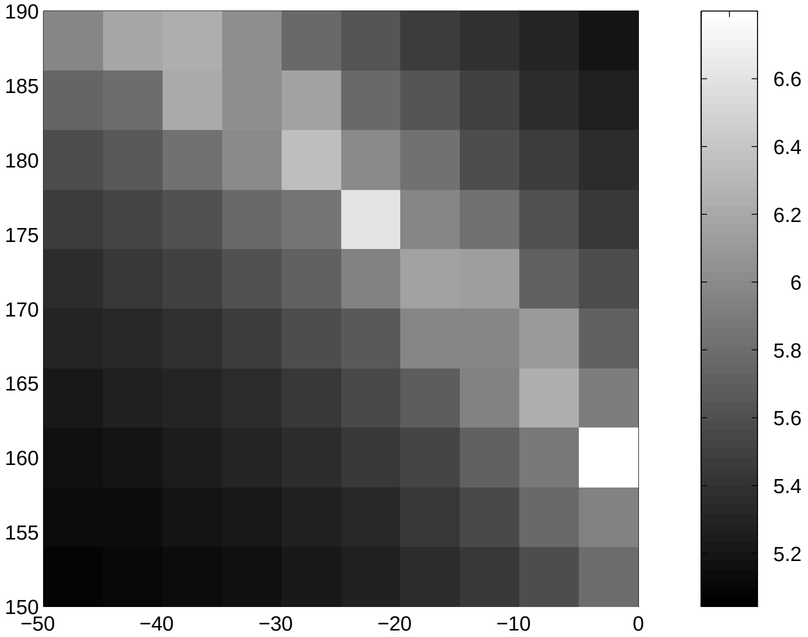

Figure 13: Tolosa matrix. General version. Zoom in the region $[-50, 0] \times [150, 190]$. $Mesh\ 10 \times 10$.

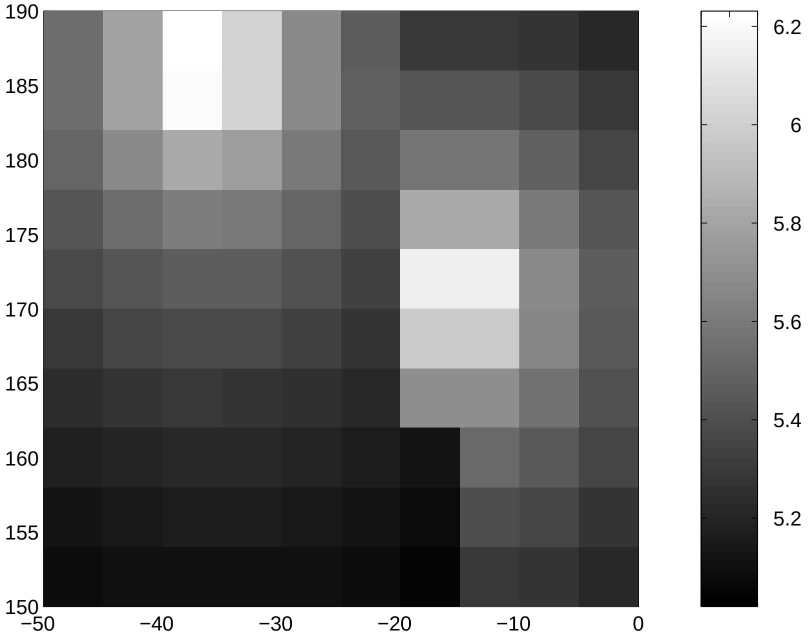

Figure 14: Tolosa matrix. Previous Point version. Orthogonality problem. Zoom in the region $[-50, 0] \times [150, 190]$. *Mesh* 10×10.

5.4 About the CPU time

For all applications, the CPU time required for the spectral portrait evaluation with the previous point version has been shown to be less than that required with the SVD method. However, this can not be taken into account because of the problem verified with the convergence. On the other hand, the general version, which is reliable, is more CPU time consuming than the SVD method for some applications. This is due to the generally slower convergence for the first eigenvalue and consequently larger basis are generated by the eigensolver.

6 Conclusion

This work describes an alternative approach to the SVD method for the evaluation of the spectral portrait. We have used a Lanczos based code to compute the smallest eigenvalue of a matrix $(A - zI)^*(A - zI)$, for distinct values of z.

We have developed two strategies :

a) a previous point one, which takes into account the eigenvector associated with the smallest eigenvalue computed on the point z previously examined,

b) a general one, which does not consider any information from the previously examined point z.

The previous point version has been shown to be faster than the SVD method. However, it is not reliable since it can yield to wrong results due to the orthogonality of eigenvectors on adjacent points. Conversely, the general version leads to results which are similar to the ones obtained by the SVD method.
However, for some applications, the general version is more CPU time consuming than the SVD method. Moreover, due to the squared conditioning of the Normal Equation approach, a sort of pigmentation can be found around singular points, corresponding to points where the eigenvalue is computed with a poor accuracy.

Therefore, it seems that an Augmented Matrix version approach would be more efficient for spectral portrait evaluations. Such an approach is better conditioned and can also benefit from the use of a Lanczos technique. Some experiments with the Augmented Matrix are currently being performed and will be discussed in forthcoming reports.

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A Description of the code

The main subprogram for the spectral portrait evaluation is `portrait.f`, which has the following characteristics :

- It defines work arrays whose dimensions are specified by the parameters `NMAX` and `MAXW`. Such parameters can be redefined by the user in order to match a particular application, as follows :
  `NMAX` must be equal to or greater than n, the dimension of the matrix.
  `MAXW` corresponds to the workspace required by the eigenvalue computation code.
- It reads the variables that define the type of the matrix to be studied, the strategy to be used and the mesh on the complex plane. It also reads the entries of the matrix.
- It calls the subroutine `readHB`, which is an interface for `READMT` from *SPARSKIT* (see Saad (1993)), for the input of matrices from the Harwell-Boeing collection.
- It defines the strategies to be used by calling either `maillage` or `maillagePP` which correspond to the general and previous point version, respectively. These subroutines are interfaces for the eigenvalue computation package. However, in any case, `maillage` is first used for the computation of $\|A\|_2$.

B User's guide

B.1 INPUT files

This section describes the input files required by the spectral portrait evaluation code, which are the followings

- `STRATEGY` : This file contains the choice for the version to be used. We recall that the Harwell-Boeing version only works with the previous point strategy. See example below.

```
H/B matrix? 0 for no, 1 for y
0
Previous Point version? 0 for no, 1 for yes
1
If H/B matrix give the name (*_rua)
no name
```

- PARAMETER : This file contains the mesh parameters and the control values for the eigenvalue package. The bounds for the real part are given by xmin and xmax while the bounds for the imaginary part are given by ymin and ymax. The partitioning of the region is defined by xmesh and ymesh.

```
Give xmin
-4.0
Give xmax
4.0
Give ymin
-1.0
Give ymax
1.0
Give xmesh
256
Give ymesh
256
Give the precision(backward error)
1.e-15
Give the size of the matrix
7
Give the maximum number of step
4
Give the number of required eigenpairs
2
Maximum number of steps for the 1-st point or restarsting (PP version)
6
Number of required eigenpairs for the 1-st point or restarsting (PP version)
4
```

- MATRIX : When the matrix does not belong to the Harwell-Boeing collection, it must be specified in this file, column by column. See example below.

```
-2.0
0.0
0.0
0.0
0.0
0.0
0.0
25.0
-3.0
0.0
0.0
0.0
```

```
0.0
0.0
0.0
10.0
2.0
0.0
0.0
0.0
0.0
0.0
3.0
15.0
0.0
0.0
0.0
0.0
0.0
3.0
3.0
15.0
3.0
0.0
0.0
0.0
3.0
3.0
3.0
10.0
-2.0
0.0
0.0
0.0
0.0
0.0
0.0
25.0
-3.0
```

B.2 OUTPUT files

This section describes the OUTPUT files which are

- `OUTPUT1` : gives the real part of each point of the mesh.

- `OUTPUT2` : gives the imaginary part of each point of the mesh.
- `OUTPUT3` : gives the value of $\|A\|_2\|(A - zI)^{-1}\|_2$ for each point of the mesh, associated with `OUTPUT1` and `OUTPUT2`.

These files will be used by the *Matlab* post-processing, in order to visualize the spectral portrait.

B.3 *Matlab* post-processing

The spectral portrait will be visualized using the *Matlab* routine `dessin.m`. After reading the OUTPUT files, this routine uses the intrinsic *Matlab* functions, `pcolor` and `colorbar`, and the subroutines `forme.m`and `reforme.m`.